Monte Carlo simulation of nematic liquid crystal in porous media: The topological constraint and surface anchoring effect

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多孔質に閉じ込められた系や不純物を含む凝縮系では、純粋な系に比べて様々な相転移現象が抑制されることが知られている。液晶における等方ーネマティック転移においても、多孔質中では不連続な一時転移を起こさなくなることが分かっている。しかしながら、液晶相は弾性的であり空間束縛を受けることにより弾性エネルギーが増大し配向欠陥が形成されるため、一般的な議論が用いることができない。例えば、この系では、外場によって平均的な配向方向を制御することができ、外場を除いた後もそれが保持されることが報告されている。これまで、不純物という形で閉じ込め効果を扱った研究した例はいくつかあったが、多孔質の構造そのものに注目したものはなく、どのように配向欠陥が束縛を受けるかなど明らかになっていない点も多く残っている。我々は様々な構造を持つ多孔質を用意し、それと配向欠陥のトポロジカルな構造との関係に着目し、メモリー効果を中心にその振舞いを調べた。相分離モデルを用いて双連結構造を用意し、その片方の相に Lebwohl-Lasher ポテンシャルで相互作用するスピンを導入し、モンテカルロシミュレーションを行った。また、図 1 は、双連結構造とその中に封入したネマティック液晶の配向欠陥を図示したものである。十分にアニールしても、液晶相の配向欠陥は消失せず残ったままであった。この配向欠陥は一意に決まるものではなく、様々な配置状態を取りうるが、それらが熱的に状態遷移することはない。大きな外場を与えると、異なる欠陥構造を持つ局所安定状態に遷移するが、その後、外場を消しても配向欠陥のトポロジーは保持されるため、一時的に印加した外場の情報を「記憶」できることが分かった。また、キュービック相など秩序度の高い多孔質を用いることで、メモリー効果の効率が高くなることも示された。

Nematic liquid crystal (LC) in porous media adopts configurations determined by the boundary conditions at the LC-solid interfaces and by the spatial distribution of topological defects. Accommodation of nematic axis according to the boundary conditions in complex porous media involves the formation of disclination lines. Previous investigations have suggested the possibility that such lines of topological defect could stably assume various trajectories, all compatible with the boundary conditions. Here we present a study of the LC topological defect in nematics confined in porous matrices of various geometries by Monte Carlo simulations with Lebwohl-Lasher potential. Our results indicate the possibility of designing highly efficient heterogeneous

LC/solid materials for optical memory. The study was first performed in realistic random bicontinuous structures resembling the porous membranes used as LC-imbibed materials in previous experiments. To realize such realistic porous structures we exploited a phase separation model, replaced one of the phases with a LC and attributed perpendicular LC anchoring at the interfaces. We find that when the LC order develops, even after long annealing, many disclination lines are left wandering through the channels to eventually close in loops. We also find that near a curved surface, a disclination line tends to align along the direction of a principle curvature. Since all channels do not necessarily have disclination lines running through them, many metastable configurations can be found. The configurations are long-lived since the energy barriers connecting them are associated to simultaneous LC rotation in entire channels, and hence much larger than thermal fluctuations. This results in strongly non-ergodic glassy behavior, analogous to a spin glass. Application of a strong external field melts the frozen defect structure and lead to different structures that do not relax into the original topology as the field is switched off. We compare such memory effect with the memory effect found in experiments on nematics in random porous media. In an effort to elucidate the physical nature of this topological multistability, we have studied the role of the symmetry and order of the porous structure. Usage of an ordered porous matrix leads, in the presence of electric fields, to the ordering of the defect structure. Particularly interesting are aligned disclination rings formed in a bicontinuous cubic. For this configuration, we find a very strong memory effect when the field is applied along certain directions of the material. Overall, two factors appear crucial in enhancing the memory effect: the existence of straight channels along the applied field (geometrical factor) and the presence of saddle like surfaces (local surface topology). Our finding may provide a physical basis for developing a memory device using topological defects of liquid crystal.

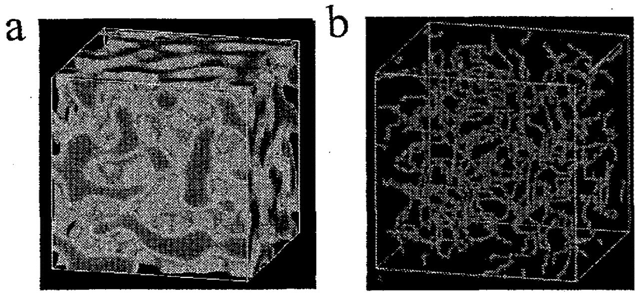

Figure 1: (a) A random bicontinuous porous medium prepared by phase separation. (b) A snapshot of remnant disclination lines in the porous medium.

References

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